QUANTUM CHEMISTRY

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QC-3.2: PARTICLE IN A BOX(2D & 3D Boxes)

PARTICLE IN A 2D-BOX

$$\mathbf{E = E_x + E_y}$$

$$= \left\{ \frac{n_x^2}{l_x^2} + \frac{n_y^2}{l_x^2} \right\} \frac{h^2}{8m} \quad ; \quad \mathbf{ZPE} = \frac{2h^2}{8ml^2} \textit{ (maximum degeneracy is two)}$$

$$\Psi = \Psi_x \Psi_y = (2/l_x)^{1/2} (2/l_y)^{1/2} \sin \frac{n_x \pi x}{l_x} \sin \frac{n_y \pi x}{l_y} = \left\{ 2/A^{1/2} \right\} \sin \frac{n_x \pi x}{l_x} \sin \frac{n_y \pi x}{l_y}$$

PARTICLE IN A 3D-BOX (Rectangular box); $(l_x \neq l_y \neq l_z)$

$$\mathbf{E_x} = n_x^2 h^2 / 8 m l_x^2$$

$$\mathbf{E = E_x + E_y + E_z}$$

$$= \left\{ \frac{n_x^2}{l_x^2} + \frac{n_y^2}{l_x^2} + \frac{n_z^2}{l_x^2} \right\} \frac{h^2}{8m} \quad ; \quad \mathbf{ZPE} = \frac{3h^2}{8ml^2} \textit{ (maximum degeneracy is six)}$$

$$\Psi_x = (2/l_x)^{1/2} \sin(n_x \pi x / l)$$

$$\Psi = \Psi_x \Psi_y \Psi_z = (2/l_x)^{1/2} (2/l_y)^{1/2} (2/l_z)^{1/2} \sin \frac{n_x \pi x}{l_x} \sin \frac{n_y \pi x}{l_y} \sin \frac{n_z \pi x}{l_z}$$

$$= (8/V)^{1/2} \sin \frac{n_x \pi x}{l_x} \sin \frac{n_y \pi x}{l_y} \sin \frac{n_z \pi x}{l_z}$$

PARTICLE IN A 3D BOX (Cubical box); $l_x = l_y = l_z = l$

$$E = (n_x^2 + n_y^2 + n_z^2) \frac{h^2}{8ml^2}$$

$$\Psi = (8/V)^{1/2} \sin \frac{n_x \pi x}{l} \sin \frac{n_y \pi y}{l} \sin \frac{n_z \pi z}{l}$$

Table: Energy & Wave function for a particle in a Cubical Box

n_x	n_y	n_z	$E = (n_x^2+n_y^2+n_z^2)\frac{h^2}{8ml^2}$	$\Psi(n_x, n_y, n_z) = (8/V)^{1/2} \sin\frac{n_x\pi x}{l} \sin\frac{n_y\pi y}{l} \sin\frac{n_z\pi z}{l}$
1	1	1	$3h^2/8ml^2$	$(8/V)^{1/2} \sin\frac{\pi x}{l} \sin\frac{\pi y}{l} \sin\frac{\pi z}{l}$
1	**1**	**2**	$\mathbf{6h^2/8ml^2}$	$\mathbf{(8/V)^{1/2} \sin\frac{\pi x}{l} \sin\frac{\pi y}{l} \sin\frac{2\pi z}{l}}$
1	**2**	**1**	$\mathbf{6h^2/8ml^2}$	$\mathbf{(8/V)^{1/2} \sin\frac{\pi x}{l} \sin\frac{2\pi y}{l} \sin\frac{\pi z}{l}}$
2	**1**	**1**	$\mathbf{6h^2/8ml^2}$	$\mathbf{(8/V)^{1/2} \sin\frac{2\pi x}{l} \sin\frac{\pi y}{l} \sin\frac{\pi z}{l}}$
1	2	2	$9h^2/8ml^2$	$(8/V)^{1/2} \sin\frac{\pi x}{l} \sin\frac{2\pi y}{l} \sin\frac{2\pi z}{l}$
2	1	2	$9h^2/8ml^2$	$(8/V)^{1/2} \sin\frac{2\pi x}{l} \sin\frac{\pi y}{l} \sin\frac{2\pi z}{l}$
2	2	1	$9h^2/8ml^2$	$(8/V)^{1/2} \sin\frac{2\pi x}{l} \sin\frac{2\pi y}{l} \sin\frac{\pi z}{l}$